Weibull Modulus Estimated by the Non-linear Least Squares Method: A Solution to Deviation Occurring in Traditional Weibull Estimation

Li, T.; Griffiths, W. D.; Chen, J.

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T. LI, W.D. GRIFFITHS, and J. CHEN

The Maximum Likelihood method and the Linear Least Squares (LLS) method have been widely used to estimate Weibull parameters for reliability of brittle and metal materials. In the last 30 years, many researchers focused on the bias of Weibull modulus estimation, and some improvements have been achieved, especially in the case of the LLS method. However, there is a shortcoming in these methods for a specific type of data, where the lower tail deviates dramatically from the well-known linear fit in a classic LLS Weibull analysis. This deviation can be commonly found from the measured properties of materials, and previous applications of the LLS method on this kind of dataset present an unreliable linear regression. This deviation was previously thought to be due to physical flaws (*i.e.*, defects) contained in materials. However, this paper demonstrates that this deviation can also be caused by the linear transformation of the Weibull function, occurring in the traditional LLS method. Accordingly, it may not be appropriate to carry out a Weibull analysis according to the linearized Weibull function, and the Non-linear Least Squares method (Non-LS) is instead recommended for the Weibull modulus estimation of casting properties.

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I. INTRODUCTION

THE Weibull distribution has been widely used to analyze the variability of the fracture properties of brittle materials for over 30 years. Fitting a Weibull distribution also later became a popular method in the prediction of the quality and reproducibility of castings.[1–3] The cumulative distribution function (CDF) of the Weibull distribution is given by[4]

$$P = 1 - \exp\left[-\left(\frac{x - x_u}{x_0}\right)^m\right], \qquad [1]$$

where P is the probability of failure at a value of x, x_u is the minimum possible value of x, x_0 is the probability scale parameter characterizing the value of x at which 62.8 pct of the population of specimens have failed, and m is the shape parameter describing the variability in the measured properties, which is also widely known as the Weibull moduli.

In a practical application, x could be substituted by the symbol σ for the properties of materials (*e.g.*, Ultimate Tensile Strength (UTS)), and the lowest possible value of property could be assumed to be 0, making $x_u = 0$, so that Eq. [1] can be re-written as a 2-parameter Weibull function:

$$P = 1 - \exp\left[-\left(\frac{\sigma}{\sigma_0}\right)^m\right]. \qquad [2]$$

There are several approaches to the estimation of the Weibull modulus in Eq. [2], with the most common methods being the Linear Least Squares method (LLS) and the Maximum Likelihood method (ML).

Many researches focused on the bias of the estimated Weibull modulus obtained by the estimation methods. Khalili and Kromp[5] recommended the ML and the LLS methods after a comparison of the ML, LLS methods, and methods of momentum. Butikofer *et al.*[6] found that the LLS method was less biased than the ML method for a small sample size. Tiryakioglu and Hudak[7] and Wu *et al.*[8] studied the best estimators for the LLS method.

However, there is still a shortcoming in the LLS method. In practice, some data points of the measured properties seriously deviate from the linear behavior in the traditional LLS method for Weibull estimation, resulting in a bad fit in the linear regression model. A good example was that of Griffiths and Lai's[2] measurement of UTS of a commercial purity "top-filled"

T. LI, W.D. GRIFFITHS, and J. CHEN are with the University of Birmingham, Birmingham B15 2TT, UK. Contact e-mail: Chenjx@bham.ac.uk
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Mg casting, as shown in Figure 1. It is clear that the data points were not randomly scattered along the fitted straight line in this linear regression, and the corresponding R^2 value was only 79.1 pct, both of which suggested that it was a bad linear fit. These outliers would exert much influence on the regression line, making the Weibull modulus deviate from its true value. This type of behavior (*i.e.,* data deviation in the lower tail) in the plots of the linearized Weibull function (Figure 1) has occurred widely and resulted in estimation bias to various degrees, of which examples can be found in References 2 and 9 through 14. Keles *et al.*[14] made a summary of this deviation occurring in the measurement of brittle materials.

When this deviation occurs, a traditional solution is to firstly eliminate a few data points before the next step of the Weibull moduli analysis,[1] because the data points in the lower tail were considered to be caused by gross pores. Nevertheless, the Weibull modulus obtained after such elimination would also neglect the effect of porosity on the quality of the castings, and could not reflect the reproducibility of the whole castings.

Currently, a popular explanation for this deviation, based on a plot of linearized Weibull CDF (Figure 1), is that the dataset may follow a 3-p/mixed Weibull distribution.[15–17] The goodness-of-fit of linear regression line (*i.e.,* R^2) was accordingly used to determine the Weibull behavior of the datasets.[18,19] Tiryakioglu[19] developed the following equation for the critical R^2 value to determine the Weibull behavior of a dataset:

$$R^2_{0.05} = 1.0637 - \frac{0.4174}{N^{0.3}}, \qquad [3]$$

where $R^2_{0.05}$ is the critical R^2 and N is the sample size. If R^2 of a linear regression was smaller than this critical value, the corresponding dataset was thought to follow a 3-p/mixed Weibull distribution.

This paper was aimed at investigating the reason for this widely reported deviation, and finding an appropriate method to estimate the Weibull modulus when such deviations occur. Preliminary work demonstrated that the widely reported deviation can be also caused by the linear transformation of the Weibull function, and a Non-LS method may be more appropriate to evaluate the Weibull modulus. Comprehensive Monte Carlo simulations and a real casting experiment were subsequently carried out to explore the reliability of the parameter estimation by Non-LS, LLS, and ML methods. It has been shown that the Non-LS method, which avoids the linear transformation, outperforms all the other methods.

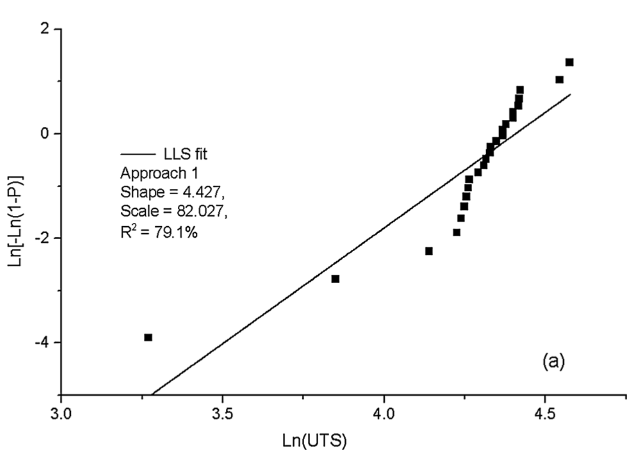

Fig. 1—Weibull estimation using the LLS method, which was published in Ref. [2] (the "Top-filled" results).

II. BACKGROUND

A. *Linear Least Squares (LLS) Methods*

The Linear Least Squares method is also known as the linear regression method. Taking the natural logarithm of Eq. [2] twice gives the linearized form of the 2-p Weibull CDF:

$$\mathrm{Ln}[-\mathrm{Ln}(1-P)] = m\mathrm{Ln}(\sigma) - m\mathrm{Ln}(\sigma_0). \qquad [4]$$

The Weibull modulus can then be determined according to the slope of a simple linear regression, (*i.e.*, ordinary least squares) of Ln $[-\mathrm{Ln}\ (1-P)]$ against $\mathrm{Ln}(\sigma)$, where the P value is assigned by a probability estimator. The probability estimators reported in the literature were generally written in the form of

$$P = \frac{i-a}{N+b}, \qquad [5]$$

where i is the rank of the data sorted in an ascending order, N is the total sample size, a and b are constants, whose values depend on the estimators used. The common estimators were summarized by Tiryakioglu and Hudak,[7] and are shown in Table I.

B. *Maximum Likelihood (ML) Method*

In statistics, the likelihood is a function of the parameters of a given observed dataset and the underlying statistical model. "Likelihood" is related to, but is not equivalent to "probability"; the former is used after the outcome data are available to describe that something that is likely to have happened, while the latter describes possible future outcomes before the data are available.

Table I. Probability Estimators Summarized by Ref. [6]

a	b	
0.5	0	Eq. [6]
0	1	Eq. [7]
0.3	0.4	Eq. [8]
0.375	0.250	Eq. [9]
0.44	0.12	Eq. [10]
0.25	0.50	Eq. [11]
0.4	0.2	Eq. [12]
0.333	0.333	Eq. [13]
0.50	0.25	Eq. [14]
0.31	0.38	Eq. [15]

The basic principles can be described as follows.[20–22] If there is a dataset of N independent and identically distributed observations, namely x_1, x_2,..., x_N, coming from a underlying probability density function $f(\theta)$. The true value of θ is unknown and it is desirable to find an estimator $\hat{\theta}$ which would be as close to θ_{true} as possible. First the joint density function for all observations can be calculated as

$$f(x_1 x_2 \ldots x_n|\theta) = f(x_1|\theta)f(x_2|\theta)\cdots f(x_n|\theta) = \prod_{i=1}^{n} f(x_i|\theta). \quad [16]$$

From a different perspective, Eq. [16] can be considered to have the observed data x_1, x_2,..., x_N, as the fixed parameters and θ as the function's variable. This will be called the likelihood function as follows

$$L(\theta|x_1 x_2 \ldots x_n) = f(x_1 x_2 \ldots x_n|\theta) = \prod_{i=1}^{n} f(x_i|\theta). \quad [17]$$

The maximum likelihood estimate (MLE) of θ can be obtained by maximizing the likelihood function given the observed data as

$$\hat{\theta}_{\text{MLE}} = \arg\max_{\theta} L(\theta|x_1 x_2 \ldots x_n). \quad [18]$$

For a Weibull estimation of castings, the likelihood function of the observed dataset, x_1, x_2,..., x_N, can be written as

$$\begin{aligned} L(m,\sigma|x_1,x_2,\ldots,x_N) &= \prod_{i=1}^{N} f(x_i|m,\sigma) \\ &= \prod_{i=1}^{N}\left(\frac{m}{\sigma}\left(\frac{x}{\sigma}\right)^{m-1}\exp\left(-\left(\frac{x_i}{\sigma}\right)^{m}\right)\right). \end{aligned} \quad [19]$$

Here $f(x_i|\, m, \sigma)$ is the probability density function of Weibull distribution. MLE of a Weibull parameter can be then obtained by maximizing Eq. [19], using Nelder–Mead method.

The estimated Weibull modulus obtained by the Maximum Likelihood method was also biased from the value of m_{true}. Khalili[5] reported that the bias level of the ML Method was higher than Eq. [6] of the linear least square method. This suggestion was also supported by the following study of References 6 and 8.

C. *Non-linear Least Squares (Non-LS) Method*

The Non-LS method has many similarities to the LLS method. The observed data are also sorted in an ascending fashion, and subsequently paired with the failure probabilities, obtained by the estimators shown in Table I. It differs from the LLS method as a non-linear regression, using a Gauss–Newton algorithm, is directly carried out to achieve the best fitted curve of a Weibull function. This method was used to estimate Weibull parameters in some other fields,[23,24] but has not been applied in the Weibull estimation of castings and brittle materials.

III. METHODS

A. *Re-analysis of Griffiths and Lai's Data*

As shown in Figure 2, the Griffiths' data shown in Figure 1 (*i.e.*, UTS of a commercial purity Mg casting produced using a top-filled running system) were re-analyzed using the Non-LS method. To compare the fitting performance, the Weibull function with the parameters obtained by the LLS method (*i.e.,* the method originally used in Griffiths and Lai's paper[2]) is also plotted in Figure 2. Residual Sum of Squares (SSR) was used to evaluate the goodness-of-fit instead of R^2 in this non-linear model (the adjusted R^2 values were also given).

According to Figure 2(a), it can be seen that the data points showed a good fit to the Non-linear regression curve (SSR = 0.0238), which is much better than the curve plotted according to the LLS estimation results (the Weibull parameters shown in Figure 1, SSR = 0.4096). There was a significant difference between the Weibull modulus estimated by the two methods (11.147 and 4.427). Therefore, although the Tiryakioglu's equation (*i.e.*, Eq. [3], $(R_{0.05})^2 = 0.9047$) rejected the Weibull behavior of this dataset, it is still not clear whether the data points follow a 2-p Weibull distribution.

According to Figure 2(b), when the Non-LS estimation result was plotted in the linearized Weibull plot (*i.e.,* solid line in Figure 2(b)), the data points showed a very bad fit to the line ($R^2 < 0$), which was much worse than the LLS estimation results (R^2 = 79.1 pct). The contradictory conclusions of Figures 2(a) and (b) suggest the following question: "Is it appropriate to determine the Weibull behavior of datasets according to the traditional linearized Weibull plot (Figure 2(b)), or the non-linear Weibull plot (Figure 2(a))?"

B. *A Shortcoming of the Linearized Form of the Weibull Function*

It should be noted that according to the estimator defined as Eq. [5], the cumulative probability in the Weibull estimation using the least square method is set to a specific value (denoted by $P_{\text{est},i}$ for the ith datum point) with the same weight for each datum point. However, in a practical process, the true cumulative probability, referred to as $P_{\text{true},i}$, is of course not necessarily equal to the estimated cumulative probability ($P_{\text{est},i}$). Bergman[25] also pointed out that it was erroneous to assume the same weight for each datum point in Eq. [5]. Thus, there is usually a difference between $P_{\text{true},i}$ and $P_{\text{est},i}$, making the estimated Weibull moduli biased.

Let $\text{DY}_{\text{non-linear},i}$ indicate the difference between the true and estimated values on the Y axis for the ith datum point in the plot of the original Weibull CDF, as shown in the following equation:

$$\text{DY}_{\text{non-linear},i} = \left|P_{\text{true},i} - P_{\text{est},i}\right|. \quad [20]$$

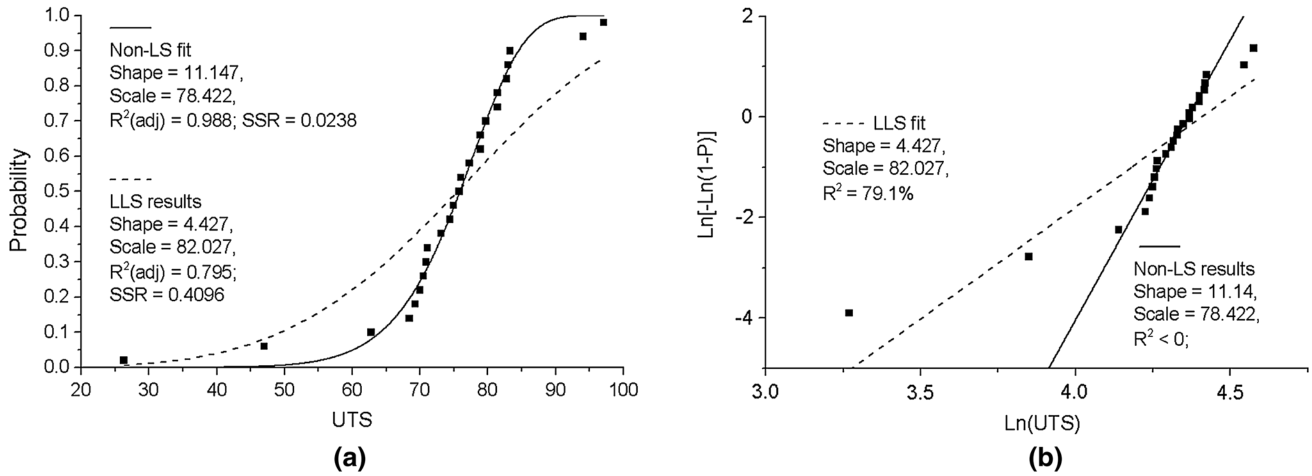

Fig. 2—(*a*) Weibull estimation of Griffiths' data shown in Fig. 1, using the Non-LS method and the LLS method. The used estimator is $P = (i - 0.5)/N$ (Eq. [6] shown in Table I). (*b*) The results of the two methods plotted in the plot of the linearized Weibull function.

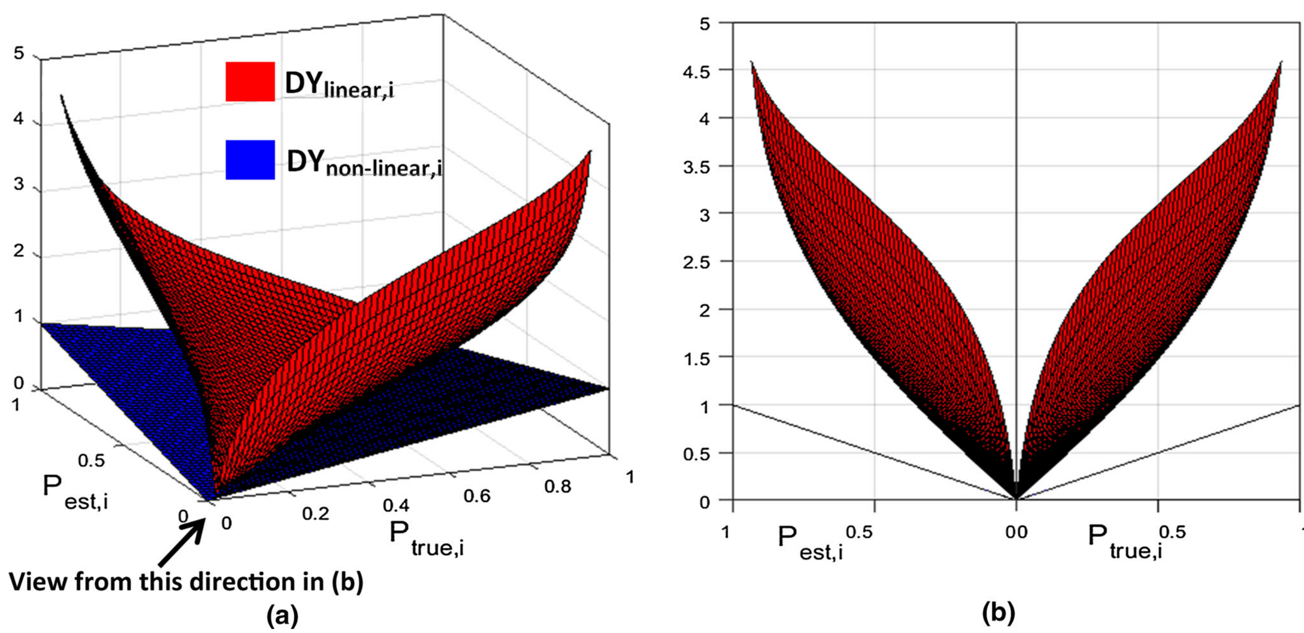

Fig. 3—(*a*) A 3D plot based on the functions of $\mathrm{DY}_{\text{linear},i}$ and $\mathrm{DY}_{\text{non-linear},i}$. (*b*) View from another direction of (a), indicating that $\mathrm{DY}_{\text{linear},i}$ is always larger than $\mathrm{DY}_{\text{non-linear},i}$.

Similarly, let $\mathrm{DY}_{\text{linear},i}$ indicate this difference on the Y axis in the plot of the linearized Weibull function (Eq. [3]), which can be calculated by the following equation:

$$\mathrm{DY}_{\text{linear},i} = \left|\mathrm{Ln}[-\mathrm{Ln}(1 - P_{\text{true},i})] - \mathrm{Ln}[-\mathrm{Ln}(1 - P_{\text{est},i})]\right|. \quad [21]$$

As shown in Figure 3, no matter how much $P_{\text{true},i}$ and $P_{\text{est},i}$ are, linear transformation can always numerically enlarge the difference between the true and estimated values on the Y axis. In other words, $\mathrm{DY}_{\text{linear},i}$ is always larger than $\mathrm{DY}_{\text{non-linear},i}$, especially when $P_{\text{est},i}$ significantly deviates from $P_{\text{true},i}$. Such an increase, in the deviation from the estimated value to the true value on the Y axis, causes a larger distance between the estimated and true positions of the data points in the linearized Weibull function plot, compared with that in the original Weibull CDF plot. Furthermore, it should be noted that the enlargement due to the linear transformation also exists in the linearized form of the 3-p Weibull function.

This enlargement level can be further described by the following enlargement factor (EF):

$$\text{Enlargement factor: EF} = \frac{\mathrm{DY}_{\text{non-linear},i}}{\mathrm{DY}_{\text{linear},i}}. \quad [22]$$

A 3D plot of this equation is shown in Figure 4. It can be seen that the EF value would be significantly small,

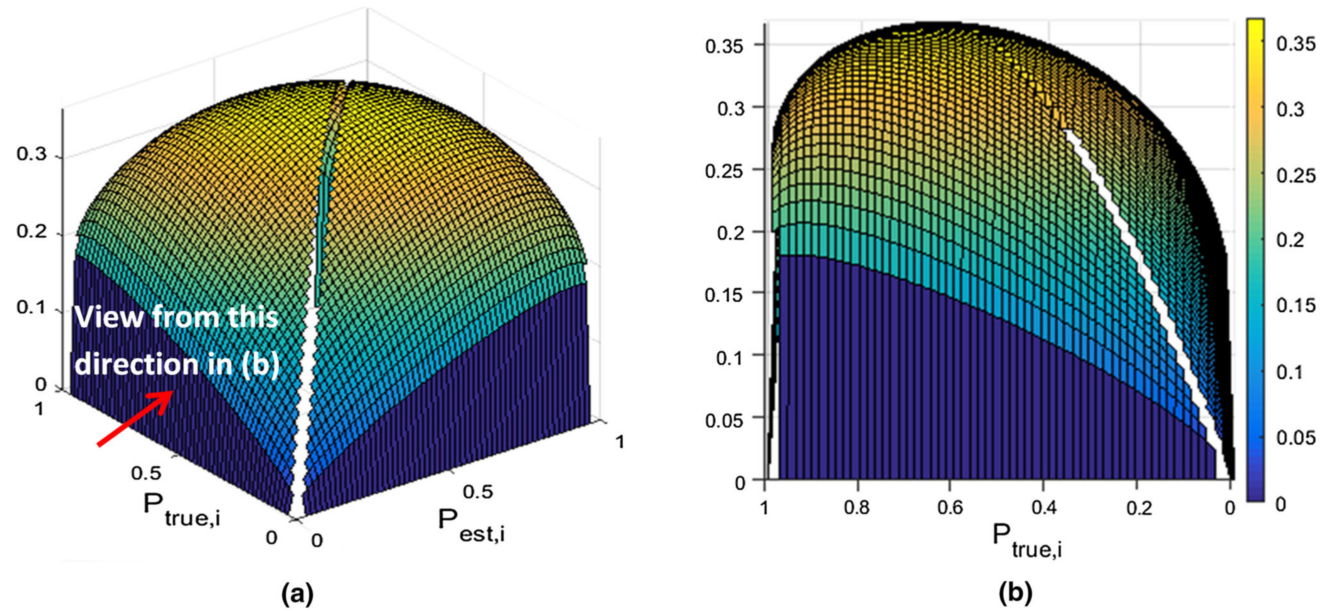

Fig. 4—(*a*) The function of the enlargement factor (EF). (*b*) View from another direction of (a), indicating the $D_{Y\text{non-linear},i}$ would be dramatically enlarged when $P_{\text{ture},i}$ is close to 0 or 1.

even close to 0, when $P_{\text{true},i}$ approaches to 0 or 1, which means that the $DY_{\text{non-linear},i}$ would be dramatically enlarged at these positions. This non-uniform enlargement is the underlying reason why it was normal to report a deviation in the lower and upper tails of a dataset in a traditional linearized Weibull plot (Figure 1).

Since the regression algorithms of the least square method (no matter linear or non-linear regression) produce the result according to the residuals (*i.e.,* the smallest Sum of Residual Squares), which is only related to the Y-coordinate, the non-uniform enlargement of $DY_{\text{linear},i}$ accordingly may result in more bias of the regression results (such as the estimated Weibull moduli). Therefore, the bad fit of the Non-LS estimation result shown in Figure 4(b) may be due to the enlargement of the difference between the true and estimated probabilities. The least square method has been accordingly used in this paper in the plot of the non-linear Weibull CDF, rather than its linearized form. This approach is the non-linear least square method (Non-LS).

C. *Examples of the Negative Effect of the Enlargement of $DY_{\text{non-linear},i}$ on Weibull Estimation*

For a further illustration of the negative effect of the enlargement of $DY_{\text{non-linear},i}$, an example has been given in Table II. This dataset was generated from a 2-p Weibull distribution with shape = 11 and scale = 60, which was close to the Non-LS estimation result of Griffiths (Figure 1). The raw data were sorted in ascending order, shown in the second column of Table II. The true cumulative probabilities ($P_{\text{true},i}$) were directly calculated from the Weibull function as listed in the third column. The estimated cumulative probability was computed according to $P_{\text{est},i} = (i - 0.5)/N$ (Eq. [6]), and has been shown in the 4th column. $DY_{\text{linear},i}$ and $DY_{\text{non-linear},i}$ were listed in the 5th and 6th columns, respectively.

Figures 5(a) and (b) show the corresponding Weibull estimation results using the Non-LS and LLS methods. The solid square points indicate $P_{\text{true},i}$, while the hollow triangle points denote $P_{\text{est},i}$. It can be seen that the deviation from the estimated value to the true value on the *Y* axis was obviously larger in the plot of the linearized Weibull function ($DY_{\text{linear},i}$ in Figure 5(b)), than in the plot of the original non-linear Weibull CDF ($DY_{\text{non-linear},i}$ in Figure 5(a)), especially when $P_{\text{true},i}$ is small. A deviation similar to that shown in Figure 1 (*i.e.,* Griffiths' data) consequently occurred in the lower tail as shown in Figure 5(b).

In addition, the Weibull behavior of this dataset was also rejected by Tiryakioglu's equation (Eq. [3]). The line plotted based on the Non-LS estimation (*i.e.*, the solid black line in Figure 5(b)) showed an extreme bad fit to the triangle points (*i.e.,* $R^2 < 0$), similar to that shown in Figure 2(b). However, this line was more close to the true function than the linear regression line.

Figure 5(c) shows the change in the enlargement factor (EF) along with $P_{\text{true},i}$, revealing that the enlargement of $DY_{\text{non-linear},i}$ was more dramatic when $P_{\text{true},i}$ is close to 0 and 1, which is consistent with Figure 4. Accordingly, the performance of the Weibull moduli estimation is poorer in the LLS method than in the Non-LS method, which can explain the different level of the goodness-of-fit in different Weibull plots as shown in Figure 2.

IV. SIMULATION PROCEDURES

To further illustrate the discussion in Section III, Monte Carlo simulations were performed in R Version

Table II. Data (Referred to as x) Generated from a Weibull Function with Shape = 11, Scale = 60

i	x	$P_{\mathrm{true},i}$	$P_{\mathrm{est},i} = (i - 0.5)/N$	$\mathrm{DY}_{\mathrm{linear},i}$	$\mathrm{DY}_{\mathrm{non\text{-}linear},i}$
1	34.0085	0.001938	0.02	0.018062	2.34314
2	34.6850	0.002406	0.06	0.057594	3.24576
3	37.1551	0.005122	0.10	0.094878	3.02130
4	42.4875	0.022199	0.14	0.117801	1.90484
5	51.1540	0.158850	0.18	0.021150	0.13734
6	51.8391	0.181473	0.22	0.038527	0.21573
7	54.0502	0.271693	0.26	0.011693	0.05155
8	54.5408	0.295427	0.30	0.004573	0.01843
9	55.1336	0.325901	0.34	0.014099	0.05221
10	55.2120	0.330076	0.38	0.049924	0.17674
11	55.3406	0.336997	0.42	0.083003	0.28175
12	55.7049	0.357082	0.46	0.102918	0.33283
13	56.6743	0.413777	0.50	0.086223	0.26074
14	57.0168	0.434843	0.54	0.105157	0.30805
15	57.8910	0.490647	0.58	0.089353	0.25148
16	58.0565	0.501496	0.62	0.118504	0.32925
17	58.2651	0.515268	0.66	0.144732	0.39860
18	58.6562	0.541344	0.70	0.158656	0.43479
19	59.7578	0.615759	0.74	0.124241	0.34242
20	60.5805	0.671011	0.78	0.108989	0.30892
21	60.8124	0.686338	0.82	0.133662	0.39136
22	61.0008	0.698679	0.86	0.161321	0.49409
23	62.7504	0.805486	0.90	0.094514	0.34101
24	63.0698	0.822946	0.94	0.117054	0.48552
25	64.0881	0.873164	0.98	0.106836	0.63899

3.3.0 (https://www.r-project.org). As shown in Figure 6, different procedures were used to investigate the bias of the estimated Weibull modulus.

For direct comparison of the different estimation methods (Figure 6(a)), random data points of sample size N were firstly generated from a 2-p Weibull function (Eq. [2]) with shape parameter = 11 (referred to as m_{true}) and scale parameter = 60 (referred to as $\sigma_{0,\mathrm{true}}$). The different approaches, listed in Table III, were used to evaluate the Weibull modulus (written as m_{est}) of the generated data.

The bias of the estimated Weibull modulus (m_{est}) was defined by the following equation,[5,7,26]

$$M = m_{\mathrm{est}}/m_{\mathrm{true}}. \quad [23]$$

M = 1 means the approach used was unbiased. In addition, since the estimated parameters are normalized by the true parameters, the setting of the scale and shape parameters are inconsequential.[5,19] This process was repeated for 20,000 times to obtain 20,000 M values. The bias level of the different approaches was evaluated by the mean of the 20,000 M values, written as M_{mean}.

To study the effect of the dramatic enlargement of $\mathrm{DY}_{\mathrm{non\text{-}linear},i}$ on Weibull moduli estimation (Figure 6(b)), the program checked whether the smallest datum of the randomly generated dataset was <30, thus making the data used for the simulation contain at least one datum point smaller than 30. This setting ensured a small value of the true probability of the first datum point ($P_{\mathrm{ture},1}$), and thus the corresponding difference between the true and estimated values on the Y axis ($\mathrm{DY}_{\mathrm{non\text{-}linear},1}$) would be dramatically enlarged in the linearized Weibull function plot, according to Figure 4 (when $P_{\mathrm{true},1}$ is close to 0).

Based on the linearized Weibull plot, Tiryakioglu *et al.*[19] developed an equation for critical R^2 (see Eq. [3]), to determine the Weibull behavior of datasets. Similarly, based on the non-linear Weibull plot, the critical SSR (referred to as SSRC) could also be calculated using a Monte Carlo simulation and the procedures shown in Figure 6(c). The SSRC obtained would be larger than the SSR value of 95 pct datasets (*i.e.,* 19,000 out of 20,000).

V. RESULTS

A. *Direct Comparison of the Estimation Approaches*

Figure 7 illustrates the results of the simulations shown in Figure 6(a). In general, the estimated Weibull modulus became closer to m_{true} with increase in sample size N. Figure 7(a) summarizes the M_{mean} obtained by the LLS and the ML methods (*i.e.*, Approaches 1 to 10 and 21 in Table III). It can be seen that Approaches 1 and 9 were relatively less biased for $N \geq 25$, and Approach 5 was the least biased approach when the sample size N was <25. This observation was consistent with the results of References 5 and 7. Figure 7(b) shows a summary of M_{mean} achieved via the Non-LS method (*i.e.,* Approaches 11 to 20 in Table III). It was obvious that Approach 12, which was the worst estimator for the LLS method (*i.e.,* Approach 2), was less biased than the other estimators using the Non-LS method, especially when the sample size was smaller than 30.

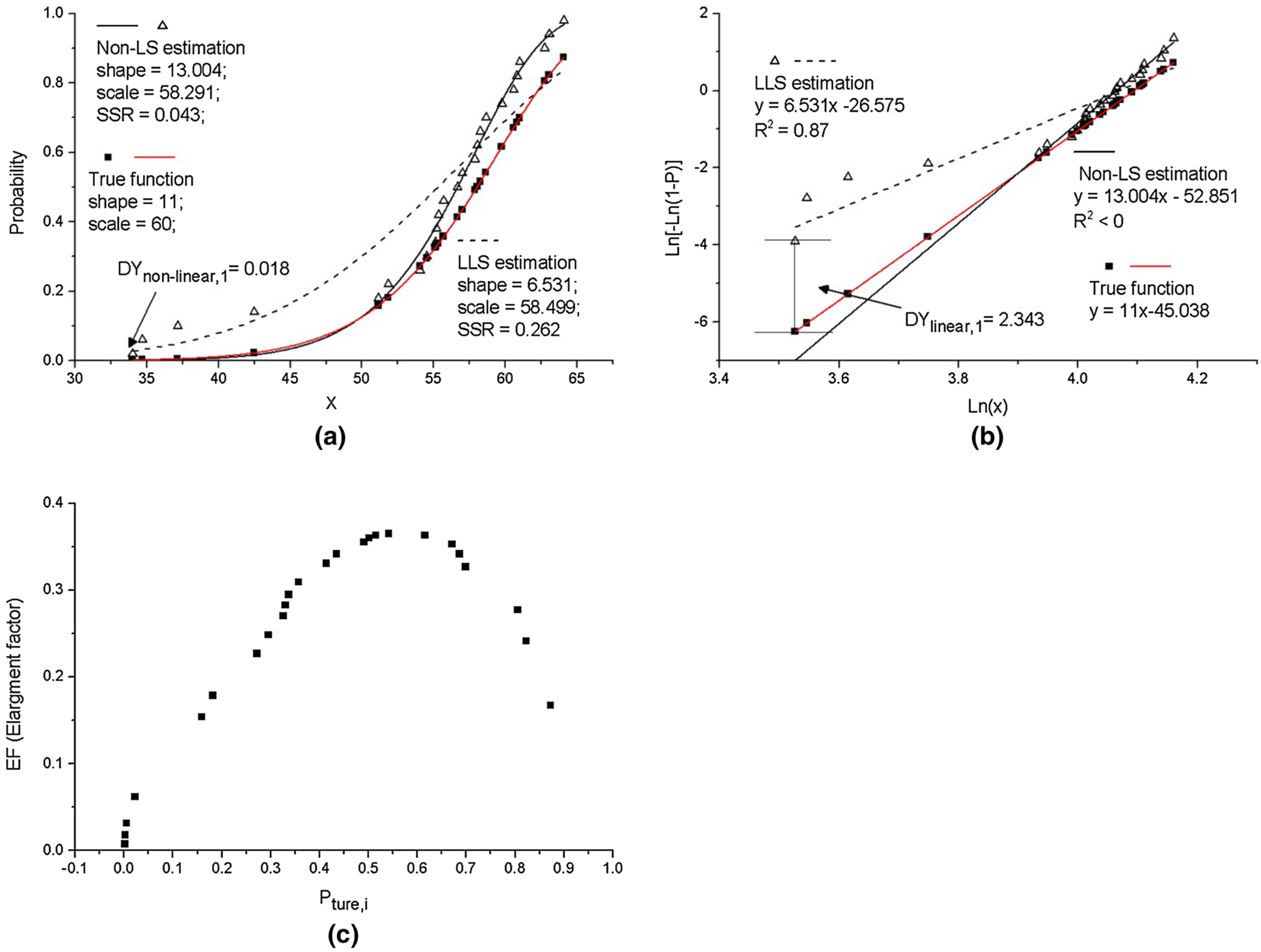

Fig. 5—(*a*) and (*b*) Weibull estimation using (a) the Non-LS and (b) LLS methods, corresponding to the data listed in Table II. The black points indicate $P_{true,i}$, while the red points denote $P_{est,i}$. (*c*) The change of EF along with $P_{ture,i}$.

For a further comparison, Approaches 1, 5, 9, and 12 were put together as shown in Figure 7(c). For $15 \leq N < 35$ and $90 \leq N$, it was clear that Approach 12 resulted in the least bias for all the sample sizes. For $35 \leq N < 90$, Approaches 1 and 12 were better than the other approaches. Figure 7(d) shows the Standard Error (SE) of M, revealing a negligible difference between the SE values of different approaches.

B. *Effect of a Dramatic Enlargement of $DY_{non\text{-}linear,i}$*

Figure 8 shows the M_{mean} of the datasets containing at least one datum point <30. As can be seen from Figure 8(a), the LLS method (*i.e.*, Approaches 1 to 10 in Table III) was seriously biased when dealing with this type of data. For $15 \leq N \leq 40$, which was the common sample size for obtaining the Weibull modulus of castings in previous publications,[2,27–29] the M_{mean} values were no more than 0.7, presenting a significant bias of the estimated Weibull modulus. In addition, even with a large sample size, such as $N = 115$, the M_{mean} values of Approaches 1 to 10 still did not exceed 0.85. Thus, it can be suggested that the LLS method is not suitable for estimating the Weibull modulus, when $P_{est.i}$ dramatically deviates from $P_{true,i}$ in the lower tail. This may explain why the data points shown in Figure 1 deviated from the linear fit.

By contrast, according to Figure 8(b), the Non-LS method (*i.e.*, Approaches 11 to 20) was significantly less biased. Even the worst approach (Approach 12) of the Non-LS method could cause a smaller bias ($M_{mean} > 0.85$, at $N = 15$) than any approaches using the LLS method ($M_{mean} < 0.8$, at $N = 115$). In addition, Approach 11 obtained the least biased estimates among all the approaches using the Non-LS methods (Approaches 11 to 20), especially when the sample size was smaller than 30.

Moreover, it should be noted that Approach 12, which was unbiased in Figure 7(b), became the most seriously biased estimator among the approaches of the Non-LS method, indicating that the bias of the approaches could be different depending on the level of the enlargement of $DY_{non\text{-}linear,i}$.

M_{mean} obtained by the ML method (Approach 21 in Table III) was also shown in Figure 8(b), but it was clear that Approach 21 was more biased for all the sample sizes examined, in contrast to the Non-LS method.

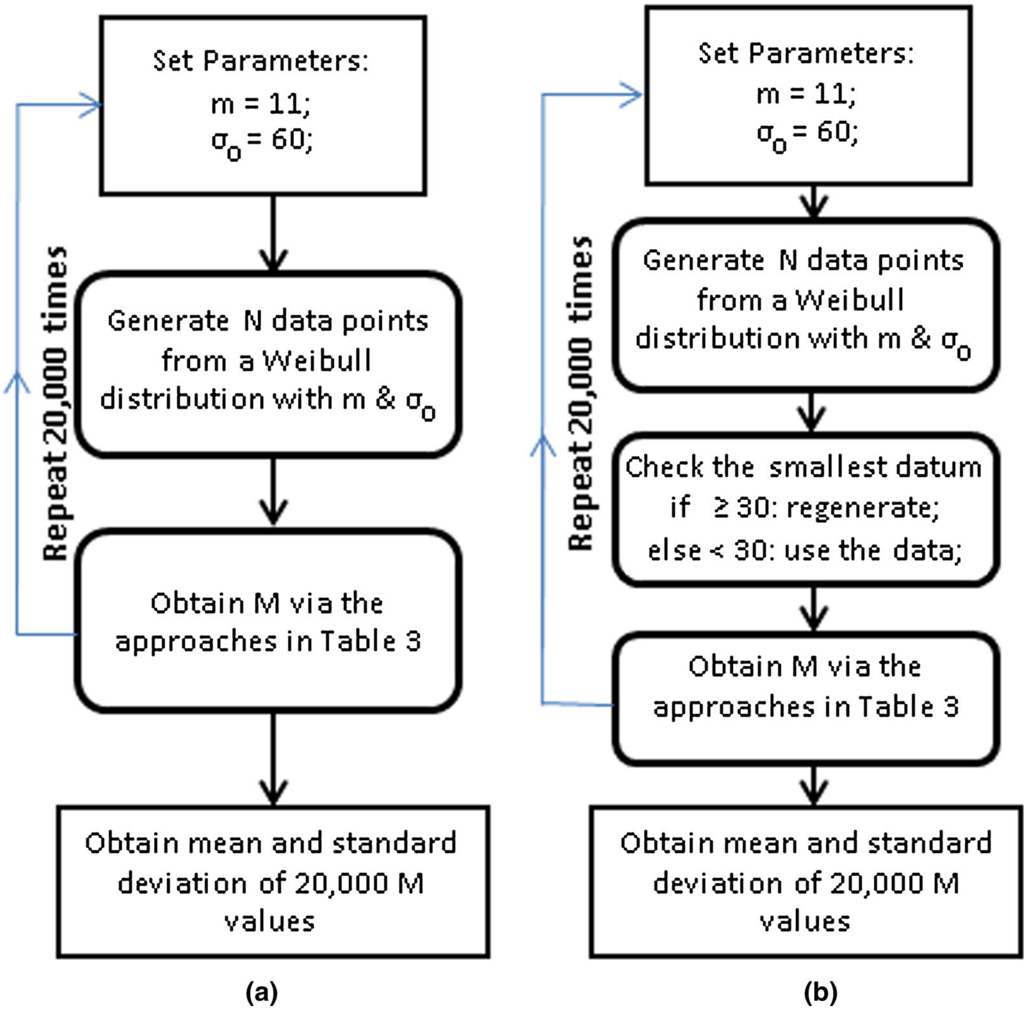

Fig. 6—Flowcharts summarizing the simulation procedures: (*a*) direct comparison of the three estimation methods; (*b*) to study the effect of the enlargement of $DY_{\text{non-linear},i}$ on Weibull estimation.

95 pct CI (confidence interval) of Approaches 1, 11, and 21 was computed under an assumption that the M values follow a standard normal distribution, as shown in Figure 8(c).

Therefore, the Non-LS method is relatively reliable, when the estimated probability ($P_{\text{est},i}$) deviated dramatically from true probability ($P_{\text{ture},i}$) in the lower tail, and Approach 11 was recommended to be the default to estimate the Weibull modulus for this type of data.

C. *Critical Sum of Residual Squares (SSRC)*

Table IV shows the SSRC values for different sample sizes. The estimator used was $P = (i - 0.5)/\text{N}$ (*i.e.*, Eq. [6] in Table I). As previously mentioned, 95 pct Weibull datasets (19,000 out of 20,000) in the simulation had a smaller SSR than SSRC. Applying this criterion to the Non-LS estimation result shown in Figure 2 ($N = 25$), it can be determined that Griffiths and Lar's data (Figure 1) follow a 2-p Weibull distribution.

However, it should be noted that this suggestion was quite different using Tiryakioglu's equation (*i.e.*, Eq. [3]), which suggested that Griffiths and Lar's data followed a 3-p/mixture Weibull distribution. In conjunction with the discussion in Section III–B, Tiryakioglu's equation may falsely reject the Weibull behavior of Griffiths' data, due to the shortcomings of the linearized Weibull function.

In addition, since the SSR value is affected by the sample size N, SSRC values of the samples having different sizes could not be directly compared with each other. Therefore, the mean sum of residual squares ($\text{SSRC}_{\text{mean}}$) can be further used to evaluate the goodness-of-fit of the non-linear regression results, as shown in the third column of Table IV and the following equation:

$$\text{SSRC}_{\text{mean}} = \text{SSRC}/N. \qquad [24]$$

The best fit curve of $\text{SSRC}_{\text{mean}}$ was computed as shown in Figure 9, which followed the formula below:

$$\text{SSRC}_{\text{mean}} = 0.06463 * N^{-0.93778}. \qquad [25]$$

Therefore, the author recommends using this equation to determine the Weibull behavior of datasets.

Table III. Approaches Using the Estimators Shown in Table I Together with LLS, Non-LS, and ML Methods

	Methods		
Estimators	LLS	Non-LS	ML
Eq. [6]	Approach 1	Approach 11	Approach 21
Eq. [7]	Approach 2	Approach 12	
Eq. [8]	Approach 3	Approach 13	
Eq. [9]	Approach 4	Approach 14	
Eq. [10]	Approach 5	Approach 15	
Eq. [11]	Approach 6	Approach 16	
Eq. [12]	Approach 7	Approach 17	
Eq. [13]	Approach 8	Approach 18	
Eq. [14]	Approach 9	Approach 19	
Eq. [15]	Approach 10	Approach 20	

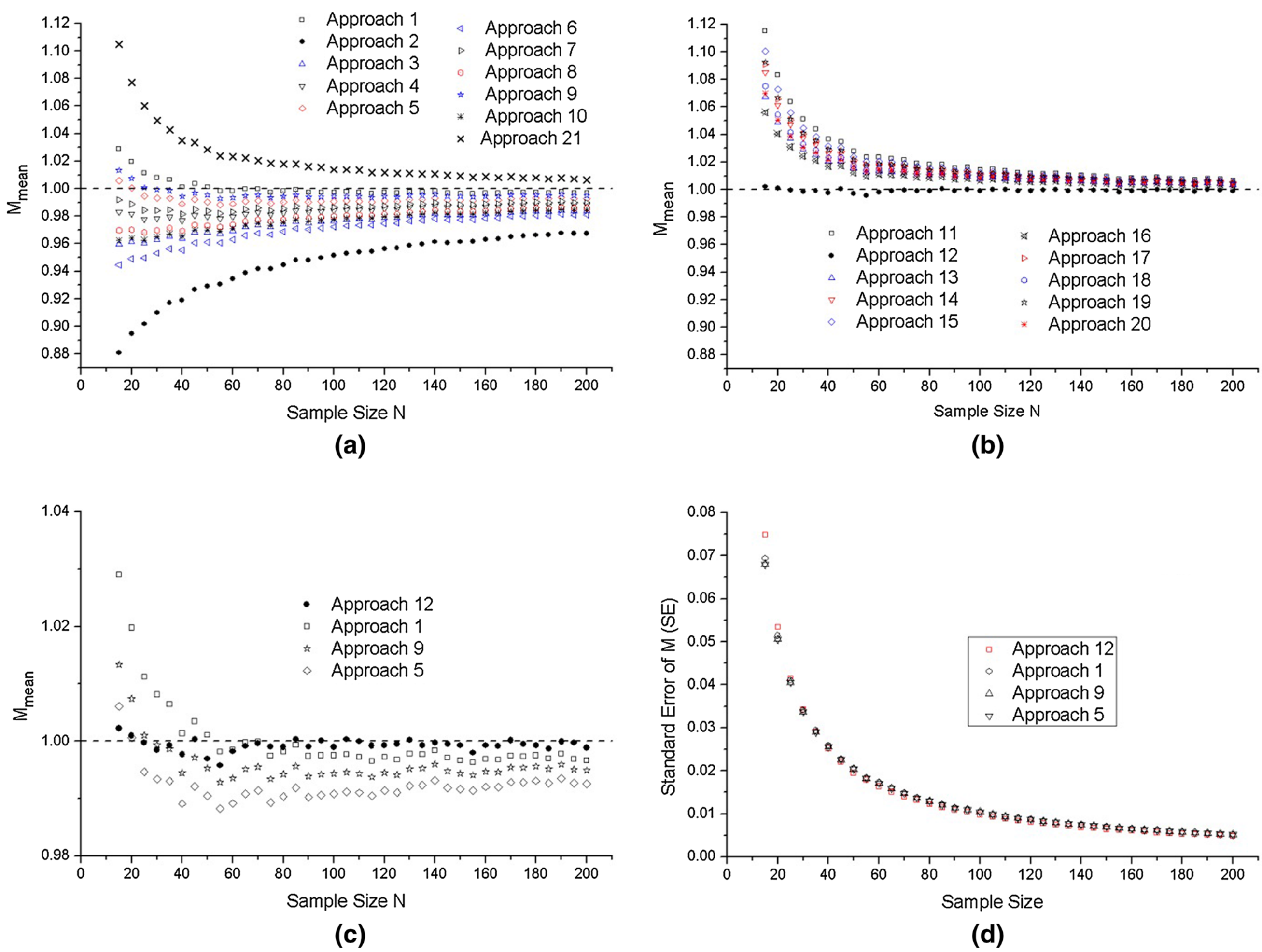

Fig. 7—M_{mean} values obtained via the approaches in Table III, (*a*) Approaches 1 to 10 and 21, (*b*) Approaches 11 to 20, for a direct comparison of the three estimation methods; (*c*) a further comparison of Approaches 1, 5, 9, and 12 shown in (a) and (b); (*d*) Standard Error (SE) of the approaches shown in (a) and (b).

D. *Practical Data from Mg-Alloy Castings*

Figure 10 shows an example of a commercial purity Mg-alloy casting. Similar to the casting shown in Figure 1, this Mg casting was also produced using a resin-bonded sand mold with a top-filled system, and the casting procedures were the same as Griffiths and Lai's work.[2] The material used was from the same batch as the Mg alloy used by Griffiths and Lai,[2] so it can be readily compared. Thus, the reproducibility of this casting was expected to be close to the results from the casting shown in Figure 1. After solidification, the casting was machined into 40 test bars and tensile strength was tested. The UTS data were used for Weibull analysis.

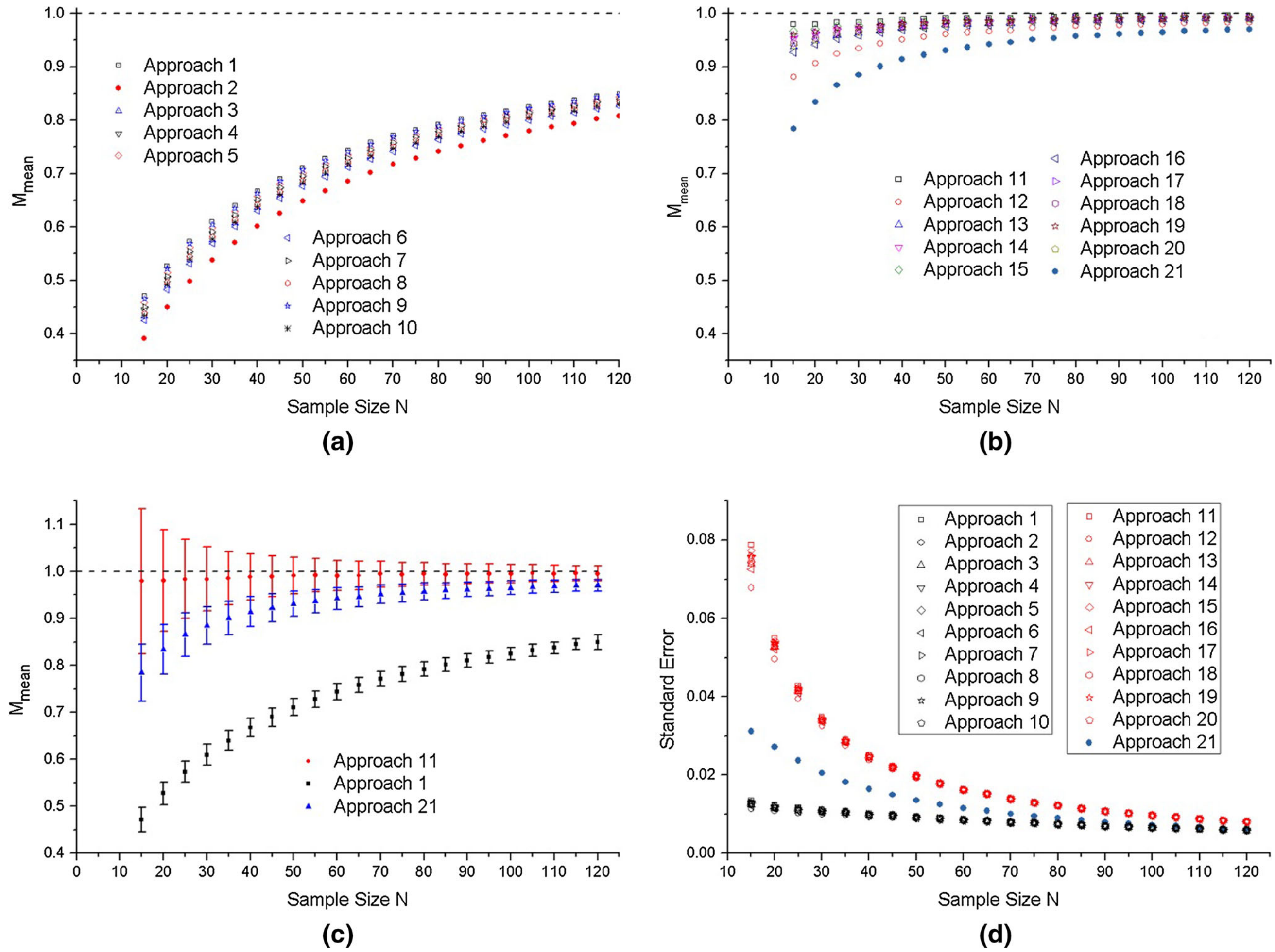

Fig. 8—M_{mean} of Approaches (*a*) 1 to 10 and (*b*) 11 to 21 applied on the dataset containing at least one datum <30. (*c*) 95 pct CI of Approaches 1, 11, 21 applied on dataset containing at least one datum <30. (*d*) Standard error of M.

Figure 10 shows the Weibull parameters evaluated using Approaches 1 and 11. It can be seen that the data points showed a good fit to the linear regression line (Figure 10(a)). In addition, in Figure 10(b), the data points showed a good fit to both the curves obtained using the Non-LS method (Approach 11, SSR = 0.0222) and the LLS method (Approach 1, SSR = 0.0265). In conjunction with Figure 7, the enlargement of $\mathrm{DY}_{\text{non-linear},i}$ in the dataset may not be dramatic. The estimated Weibull moduli (11.7 and 11.4) were close to the Non-LS estimation results shown in Figure 1, rather than the LLS estimation results.

As previously mentioned, this casting process (*i.e.*, the casting shown in Figure 10) is the same as the Griffiths and Lai's casting process (*i.e.*, the casting shown in Figure 2), and thus the estimated Weibull modulus shown in Figure 10 should be close to the true Weibull modulus of Griffiths and Lai's casting. Therefore, the Weibull modulus shown in Figure 10 could be used as the reference value to determine which Weibull modulus (*i.e.*, the LLS and Non-LS estimation results) in Figure 2 was closer to the true value. Based on the comparison between Figures 2 and 10, it can be suggested that the Non-LS estimation result shown in Figure 2 (*i.e.*, m = 11.14) is closer to the true Weibull modulus than the LLS estimation result (*i.e.*, m = 4.4). The Non-LS method is accordingly more appropriate to estimate the Weibull modulus of Griffiths and Lai's data.

In addition, this comparison (Figures 10 and 2) further revealed that the SSRC method (Figure 9) may be more appropriate to interpret Griffiths and Lai's data, while Tiryakioglu's equation (Eq. [3]) will falsely interpret this dataset to be a 3-p Weibull distribution.

Figure 11 shows an example of results from an AZ91 casting, produced in the same way as the cast test bar results shown in Figure 10. As shown in Figure 11(a), the data points deviated from the linear regression line, and the corresponding R^2 was smaller than the critical R^2 suggested by Eq. [3] [$(R_{0.05})^2$ = 0.9256), rejecting the Weibull behavior of this dataset. However, according to the non-linear Weibull plot (Figure 11(b)], there was a clear difference between curves obtained by Approaches 1 (the LLS method) and 11 (the Non-LS method). The curves obtained by Approach 11 have an SSR value smaller than the critical SSR (SSRC = 0.0816979,

Table IV. SSRC Values; the Estimator Used is $P = (i - 0.5)/N$

N	SSRC	$SSRC_{mean}$
15	0.0756771	5.0451E−03
20	0.0784904	3.9245E−03
25	0.0797666	3.1907E−03
30	0.0802094	2.6736E−03
35	0.0818855	2.3396E−03
40	0.0816979	2.0424E−03
45	0.0832347	1.8497E−03
50	0.0826510	1.6530E−03
55	0.0837245	1.5223E−03
60	0.0829798	1.3830E−03
65	0.0834890	1.2844E−03
70	0.0831899	1.1884E−03
75	0.0844495	1.1260E−03
80	0.0846093	1.0576E−03
85	0.0842047	9.9064E−04
90	0.0849502	9.4389E−04
95	0.0840484	8.8472E−04
100	0.0846551	8.4655E−04
105	0.0833319	7.9364E−04
110	0.0842549	7.6595E−04
115	0.0845723	7.3541E−04
120	0.0838167	6.9847E−04

Table IV), suggesting the data followed a 2-p Weibull distribution. This different judgment of Weibull behavior is similar to that found in the estimation of Griffiths and Lai's data (Figure 2), and the dataset may be falsely interpreted in the linearized Weibull plot.

VI. DISCUSSION

A. *Determination of Weibull Behavior of Datasets*

Figure 3 indicates that the difference between the estimated and true cumulative probabilities of data points ($DY_{non\text{-}linear,i}$) would be significantly enlarged due to the linear transformation of the Weibull function. Figure 4 further reveals that this enlargement level was not uniform: the enlargement could be more dramatic in the lower and upper tails (*i.e.,* when $P_{true,i}$ is close to 0 or 1).

According to the Weibull analysis of example data (Figures 2 and 5), the non-uniform enlargement of $DY_{non\text{-}linear,i}$ can affect the judgement of the Weibull behavior of datasets. The re-analysis of Griffiths' data (Figure 2) and the corresponding SSRC value (Table IV) indicated that it may not be necessarily correct to reject the Weibull behavior of datasets, according to the goodness-of-fit of the linear regression line (Eq. [3]). It should be noted that if a significant enlargement of $DY_{non\text{-}linear,i}$ occurred in the lower tail (*i.e.,* the first few data points), even a dataset generated from a Weibull distribution would probably present a bad fit to the linear regression line, as shown in Figure 5(b).

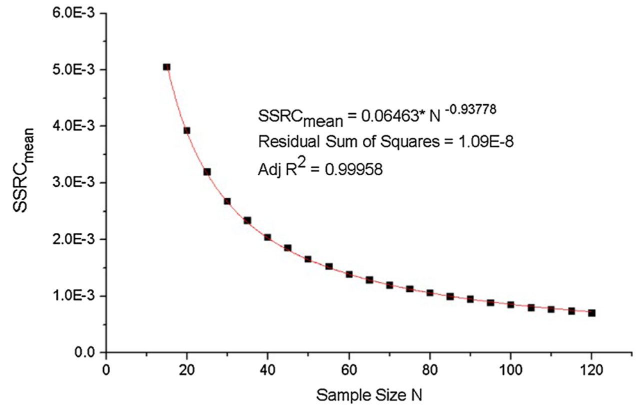

Fig. 9—$SSRC_{mean}$ for different sample sizes.

The experimental result (Figure 10) further showed the dataset of a top-filled commercial purity Mg casting followed a 2-p Weibull distribution, according to both R^2 and SSR. In addition, both of the LLS and Non-LS results in Figure 10 were close to the Non-LS estimation result of Griffiths and Lai (Figure 2), which further supported the reliability of the Non-LS estimation. Figure 11 shows a further example that the dataset may be falsely interpreted.

Therefore, the non-uniform enlargement of $DY_{non\text{-}linear,i}$ is an underlying reason for the deviation of the data points widely found in previous publications.[2,9–13] Previous researchers suggested that this deviation could be due to the nature of the physical flaws (*i.e.*, defects, such as porosity, low melting point intermetallic compounds, and segregation) in the material,[14,30] and the corresponding data points were interpreted to follow an underlying 3-p or mixed Weibull distribution.[15–17] However, more analysis (Eq. [25]) is still required to distinguish what is the actual reason of the deviation. The simulation results (Figure 5) and experimental results (Figures 2 and 10) indicated that a deviation caused by the non-uniform enlargement of $DY_{non\text{-}linear,i}$ could be falsely interpreted to be due to physical flaws (*i.e.,* 3-p/mixed Weibull distribution). This misunderstanding may exist in previous researches.

B. *Effect of Weibull Modulus Estimation*

The results of the Monte Carlo simulations demonstrated that the non-uniform enlargement of $DY_{non\text{-}linear,i}$ resulted in a greater bias in the Weibull modulus estimation. When the difference between $DY_{linear,i}$ and $DY_{non\text{-}linear,i}$ was not necessarily large (Figure 7), the Non-LS method was slightly less biased than the LLS method. However, when high enlargement of $DY_{non\text{-}linear,i}$ occurs in the lower tail (Figure 5), the Non-LS method has a considerable merit over the LLS method.

It is therefore recommended that the plot of the original non-linear Weibull CDF and the Non-LS

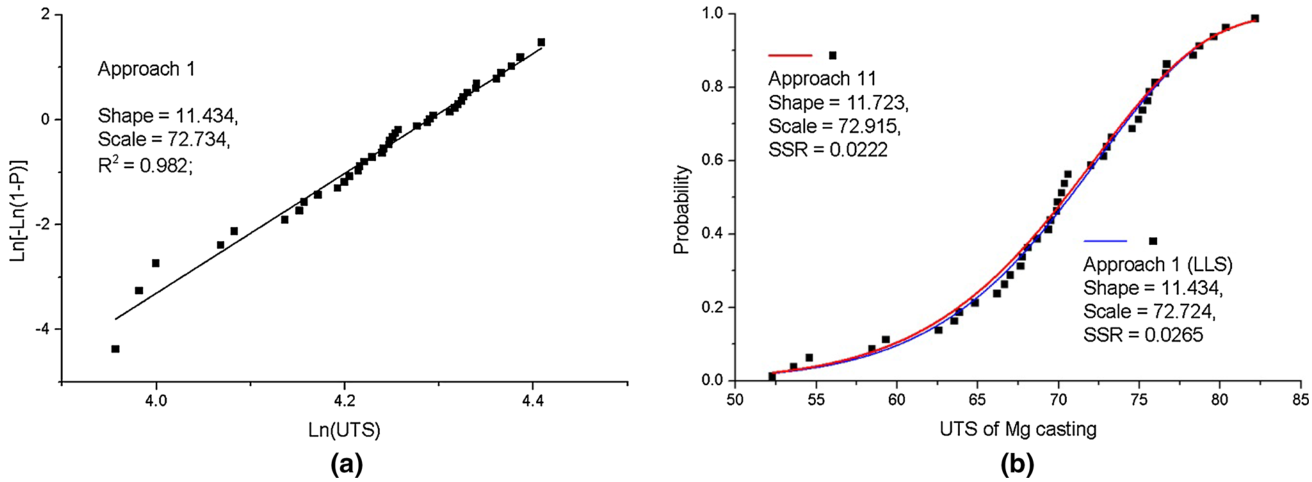

Fig. 10—Weibull estimation of UTS of the commercial pure Mg casting produced by the author. (*a*) LLS estimation, (*b*) Non-LS estimation.

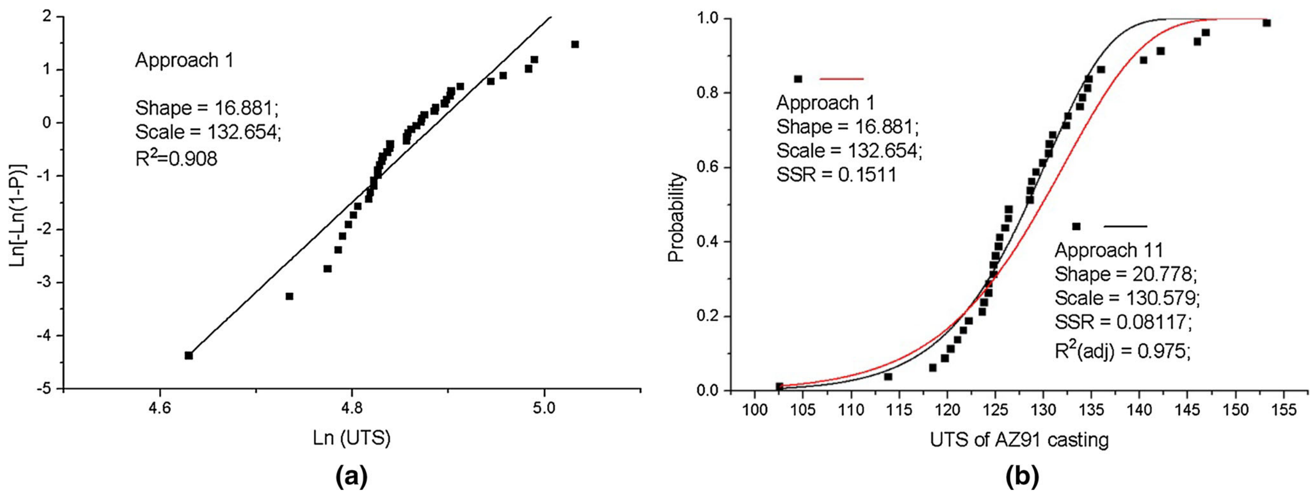

Fig. 11—Weibull estimation of UTS of the AZ91 casting produced by the author. (*a*) LLS estimation, (*b*) Non-LS estimation.

method, which avoids the linear transformation, should be used for the Weibull analysis of material properties.

VII. CONCLUSION

1. It has been demonstrated that the difference between the estimated and true cumulative probabilities of data points can be dramatically enlarged in the lower and upper tails, due to the linear transformation in the traditional Weibull modulus estimation using the LLS method.
2. Such an enlargement is an underlying reason of the deviation from the linear regression line, which was previously widely reported and interpreted to be due to physical flaws contained in the brittle and metal materials.
3. It is therefore not necessarily correct to reject the Weibull behavior of a dataset, according to the goodness-of-fit of the linear regression line, such as R^2.
4. The Non-LS method, which is demonstrated to be less biased compared with both the LLS and ML methods, is recommended for the Weibull modulus estimation.

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